Week 11: Monday, Apr 4

Problem du jour

Suppose f is twice continuously differentiable and $|f''(x)| < c$ for some modest value of c. How could I efficiently compute

$$\phi(k) = \int_0^1 f(x) \cos(kx) \, dx$$

when k is very large?

Answer: A numerically-oriented approach is Filon's method, which approximates f by a quadratic (or possibly by quadratics over panels). Integrating a quadratic times a cosine is an exercise in integration by parts.

Another approach is to write an asymptotic expansion in powers of k^{-1} using integration by parts:

$$\begin{aligned} \int_0^1 f(x) \cos(kx) \, dx &= k^{-1} f(x) \sin(kx) \Big|_0^1 - \int_0^1 k^{-1} f'(x) \sin(kx) \, dx \\ \int_0^1 f'(x) \sin(kx) \, dx &= - k^{-1} f'(x) \cos(kx) \Big|_0^1 + \int_0^1 k^{-1} f''(x) \sin(kx) \, dx \end{aligned}$$

Substituting the second expression into the first, we have

$$\int_0^1 f(x) \cos(kx) \, dx = \frac{f(1) \sin(k)}{k} + O(k^{-2}).$$

This would be a more classical asymptotic approximation.

Centered differences

Suppose f is a smooth function, and we know $f(0)$, $f(h)$, and $f(-h)$. How could we estimate $f'(0)$? There are two standard approaches to deriving a formula: interpolation, and the method of undetermined coefficients. Let us see how each works, starting with interpolation.

The Lagrange form of the polynomial interpolating f at 0, h, and $-h$ is

$$p(x) = f(-h) L_{-h}(x) + f(0) L_0(x) + f(h) L_h(x),$$

where the Lagrange polynomials are

$$\begin{aligned} L_{-h}(x) &= \frac{1}{2h^2}x(x+h) \\ L_0(x) &= \frac{1}{h^2}(x-h)(x+h) \\ L_h(x) &= \frac{1}{2h^2}x(x-h) \end{aligned}$$

We can now approximate $f'(0)$ by $p'(0)$, where

$$p'(0) = f(-h)L_{-h}'(0) + f(0)L_0'(0) + f(h)L_h'(0) = \frac{f(h)-f(-h)}{2h}.$$

Because $p(x)$ is a quadratic polynomial interpolant, we know $f(x) - p(x) = O(h^3)$ near $x = 0$, and can differentiate to find $f'(0) - p'(0) = O(h^2)$.

Now, suppose that we forgot about interpolation, and just asked what combination of $f(0)$, $f(h)$, and $f(-h)$ would give us the highest-order approximation to $f'(0)$. That is, we want to find c_-, c_0, and c_+ such that

$$g(h) = c_- f(-h) + c_0 f(0) + c_+ f(h) = f'(0) + O(h^p)$$

where p is as large as possible. If we Taylor expand f about zero, we have

$$\begin{aligned} g(h) =& (c_- + c_0 + c_+)f(0) + \\ & (c_+ - c_-)(f'(0)h + f^{(3)}(0) \\ & (c_+ + c_-)f''(0)h^2/2 \\ & (c_+ - c_-)f^{(3)}(0)h^3/6 \\ & (c_+ + c_-)f^{(4)}(0)h^4/24 + O(h^5)) \end{aligned}$$

In order to get that $g(h) \to f'(0)$ as $h \to 0$, we at least need

$$\begin{aligned} c_- + c_0 + c_+ &= 0 \\ c_+ - c_- &= h^{-1} \end{aligned}$$

But this is only two equations for three variables, so we can add an equation to increase the order of accuracy:

$$c_+ + c_- = 0.$$

These three equations yield the solution

$$c_+ = c_- = \frac{1}{2h}, \quad c_0 = 0,$$

and we can also write down the approximation error:

$$\frac{f(h) - f(-h)}{2h} - f'(0) = f^{(3)}(0)h^2/6 + O(h^4).$$

Panel integration

Suppose we want to compute the integral

$$\int_a^b f(x)\,dx$$

In estimating a derivative, it makes sense to use a locally accurate approximation to the function around the point where the derivative is to be evaluated. But if f is at all interesting on the interval $[a, b]$, it probably does not make sense to approximate the integral of f by integrating a quadratic interpolant. On the other hand, f may be approximated quite well by a quadratic interpolant on small subintervals, so it may make sense to define a mesh of points

$$a = a_0 < a_1 < a_2 < \ldots < a_n = b$$

and to then compute

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{a_i}^{a_{i+1}} f(x)\,dx,$$

where the integrals on each panel $[a_i, a_{i+1}]$ involves a local polynomial approximation. Let us now turn to a method to compute these panel integrals.

Simpson's rule

Now, suppose we do exactly the same manipulations we used to find the centered difference approximation, but aim at coming up with an integration rule. That is, given $f(-h)$, $f(0)$, and $f(h)$, how can we estimate $\int_{-h}^{h} f(x)\,dx$?

Again, we can derive the same answer by either interpolation or by the method of undetermined coefficients. Let's use interpolation first:

$$\begin{aligned}
\int_{-h}^{h} f(x)\,dx \approx & \int_{-h}^{h} p(x)\,dx \\
=& \int_{-h}^{h} \left[f(-h)L_{-h}(x) + f(0)L_0(x) + f(h)L_h(x) \right]\,dx \\
=& w_- f(-h) + w_0 f(0) + w_+ f(h), \\
w_- =& \int_{-h}^{h} L_{-h}(x)\,dx = h/3 \\
w_0 =& \int_{-h}^{h} L_0(x)\,dx = 4h/3 \\
w_+ =& \int_{-h}^{h} L_h(x)\,dx = h/3.
\end{aligned}$$

What about the method of undetermined coefficients? Let's start by integrating a Taylor expansion of f about 0:

$$\int_{-h}^{h} f(x)\,dx = 2\left[f(0)h + f''(0)h^3/6 + f^{(4)}(0)h^5/120 + O(h^7) \right]$$

We want to match terms in this Taylor expansion to the terms in the Taylor expansion of a linear combination of $f(-h)$, $f(0)$, and $f(h)$:

$$\begin{aligned}
I(h) =& c_- f(-h) + c_0 f(0) + c_+ f(h) \\
=& (c_- + c_0 + c_+) f(0) + (c_+ - c_-) f'(0)h + (c_+ + c_-) f''(0)h^2/2 \\
& + (c_+ - c_-) f^{(3)}(0)h^3/6 + (c_+ + c_-) f^{(4)}(0)h^4/24 + O(h^5)
\end{aligned}$$

If we match the constant, linear, and quadratic terms between the two expansions, we have

$$\begin{aligned}
c_- + c_0 + c_+ &= 2h \\
c_+ - c_- &= 0 \\
c_+ + c_- &= 2h/3
\end{aligned}$$

Solving gives us $c_+ = c_- = h/3$ and $c_0 = 4h/3$, and

$$\int_{-h}^{h} f(x)\,dx - I(h) = O(h^5).$$

A brief digression on changing variables

How do I get from a rule on the domain $[-h, h]$ to a rule on the domain $[a_i, a_{i+1}]$? Define $h = (a_{i+1} - a_i)/2$ and $a_{i+1/2} = (a_{i+1} + a_i)/2$. Then we can define $x = a_{i+1/2} + z$, and since $dx/dz = 1$, the change of variables formula gives

$$\int_{a_i}^{a_{i+1}} f(x)\, dx = \int_{-h}^{h} f(a_{i+1/2} + z)\, dz.$$

For example, Simpson's rule on the interval $[a_i, a_{i+1}]$ is

$$\int_{a_i}^{a_{i+1}} f(x)\, dx = \frac{b-a}{6} \left[f(a_i) + 4f(a_{i+1/2}) + f(a_{i+1}) \right].$$

Newton-Cotes rules

Simpson's rule is a member of the family of *Newton-Cotes* rules based on interpolation over a uniform mesh. The first three Newton-Cotes rules are

1. Midpoint: $\int_{-h}^{h} f(x)\, dx \approx 2hf(0)$
2. Trapezoidal: $\int_{-h}^{h} f(x)\, dx \approx h\,[f(-h) + f(h)]$
3. Simpson's: $\int_{-h}^{h} f(x)\, dx \approx h/3\,[f(-h) + 4f(0) + f(h)]$

The midpoint and trapezoidal rules have order $O(h^3)$ per panel, and Simpson's rule has $O(h^5)$ per panel. If the panel sizes are fixed, we generally have $O(1/h)$ panels to cover the domain $[a, b]$, so the absolute error in approximating an integral by composite midpoint or trapezoidal integration is $O(h^2)$, and the error for composite Simpson's rule is $O(h^4)$.

In general, n-point Newton-Cotes rules exactly integrate polynomials of degree $n - 1$ if n is even, degree n if n is odd (the degree of polynomial we integrate exactly is called the degree of the quadrature rule). Newton-Cotes rules with more than three or four points are uncommon in practice; for $n \geq 11$, the Newton-Cotes rules always have at least one negative weight, and cancellation causes problems in finite precision. Instead, Newton-Cotes rules are usually used in panel integration schemes, often with adaptive panel sizes based on local error estimates.

Error estimates

We have already seen one approach to writing a formula for the error in a quadrature rule: Taylor expand everything in sight, and get a formula involving high-order derivatives of f. Unfortunately, we may not always have easy access to bounds on the derivatives of f. In practice, we would therefore usually estimate the error by comparing the results of two integration rules with different errors over a panel.

For example, on $[-h, h]$, let us write the integral, the midpoint rule, and the trapezoidal rule as

$$\begin{aligned} I[f] &= \int_{-h}^{h} f(x)\,dx = 2hf(0) + f''(0)h^3/3 + O(h^5) \\ Q_M[f] &= 2hf(0) \\ Q_T[f] &= h\left[f(-h) + f(h)\right] = 2hf(0) + f''(0)h^3 + O(h^5). \end{aligned}$$

The error in the midpoint rule and the trapezoidal rule are thus

$$\begin{aligned} Q_M[f] - I[f] &= -f''(0)h^3/3 + O(h^5) \\ Q_T[f] - I[f] &= 2f''(0)h^3/3 + O(h^5). \end{aligned}$$

The error in the trapezoidal rule is thus about twice the size of the error in the midpoint rule. Moreover, we can estimate $Q_M[f] - I[f]$ even if we don't have direct access to the integral $I[f]$:

$$Q_M[f] - I[f] = (Q_M[f] - Q_T[f])/3 + O(h^5).$$

Note that this suggests we could get a more accurate formula by correcting $Q_M[f]$ with our estimate of the error:

$$I[f] = Q_M[f] - (Q_M[f] - Q_T[f])/3 + O(h^5).$$

But note that

$$Q_M[f] - (Q_M[f] - Q_T[f])/3 = \frac{h}{3}\left[f(-h) + 4f(0) + f(h)\right],$$

which is just Simpson's rule.